Strain and Stress in a Thin Film $YBa_2Cu_3O_x$ Bicrystal Grain Boundary on $SrTiO_3$ Substrate Studied by X-ray Micro-Diffraction

W.A. Caldwell[1], N. Tamura[1], R.S. Celestre[1], A.A. MacDowell[1], H.A. Padmore[1], and J.R. Patel[1,2]
[1]Advanced Light Source, Ernest Orlando Lawrence Berkeley National Laboratory,
University of California, Berkeley, California 94720, USA
[2]SSRL/SLAC, Stanford University, P.O. Box 43459, Stanford CA 94309, USA

INTRODUCTION

Grain boundaries are important in the electrical transport properties of high-T_c cuprate superconductors. $YBa_2Cu_3O_x$ superconducting devices take advantage of good transport behavior to make wires and use the poor transport (weak link) behavior to make Josephson junction devices [1]. Critical current densities are lower across the grain boundaries by orders of magnitude compared with the values in the bulk of single crystals [2]. The amount of misorientation of neighboring grains is an important parameter in determining the critical current density. In [001] tilt boundaries, one of the simplest grain boundaries, critical current densities drop markedly above 10 degrees [3]. High-resolution electron microscopy has shown that this misorientation angle, which corresponds to the transition from strong to weak intergrain coupling, occurs at the point of overlap of Cu-rich dislocation cores, indicating that the dislocation cores along the grain boundary are responsible for the weak-link behavior [4].

The purpose of this work is to probe the strain/stress of two $YBa_2Cu_3O_x$ bicrystal films near the grain boundary using x-ray microdiffraction in order to visualize the strain/stress fields caused by the dislocation cores at the grain boundary.

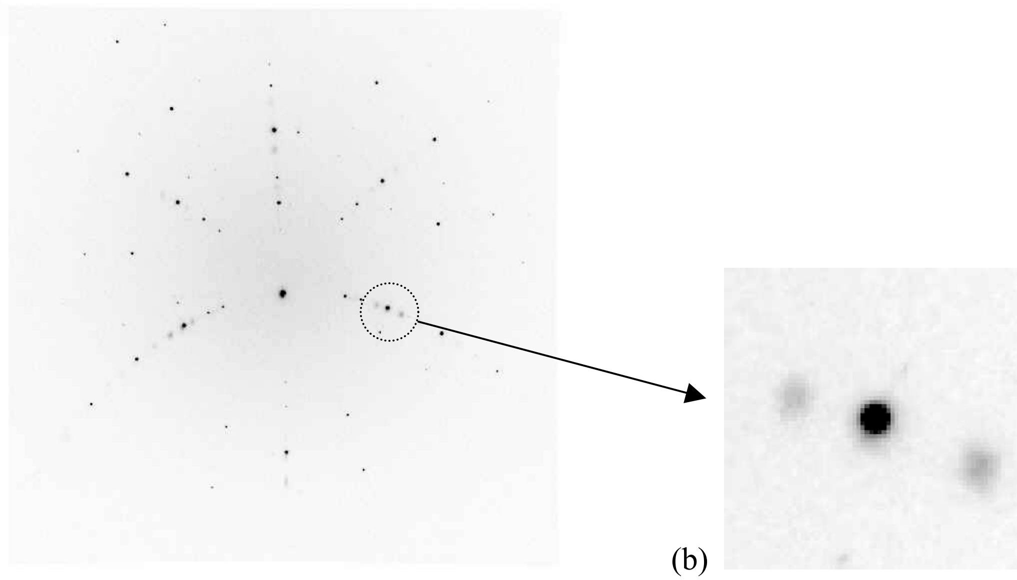
EXPERIMENTAL

The samples consist of two $YBa_2Cu_3O_x$ bicrystal samples both with [001] tilt boundaries: one with a 36° tilt (high-angle, weak-link) boundary and the other with a 10° tilt (transition between strong coupling and weak-link) boundary. Both film samples are 260 nm thick and were deposited epitaxially in a controlled (high purity - O_2) environment on $SrTiO_3$ bicrystal substrates and post-growth oxygenated at 420° C for 1 hour prior to removal from the growth chamber.

Oxygen content of our samples were determined from T_c measurements and then used to determine the stress free lattice parameters according to established reference relations [5]. White-beam Laue patterns in reflection mode at beamline 7.3.3 at the Advanced Light Source were taken and automatically indexed using a custom code (X-MAS) developed onsite. The X-ray microdiffraction end station on beamline 7.3.3 has the capability of providing high flux within a beam size of approximately 1 x 1 micron. Its setup has been described elsewhere [6].

RESULTS

Measurements were taken in 1 micron steps to make a raster scan of 30 microns across the bicrystal grain boundary and 10 microns parallel to this boundary for both samples. Additionally, finer scans were made on the 10° sample with 0.5 micron steps of 10 microns by 10 microns and also with 0.25 micron steps of 2 microns by 2 microns. A sample diffraction pattern is shown in Figure 1. The geometrical parameters (sample-detector distance, center channel position and



(a) (b)

Figure 1. (a) White-beam Laue pattern of $YBa_2Cu_3O_7$ thin film on $SrTiO_3$ bicrystal substrate. (b) The most intense spots are due to the substrate (center of enlarged image). The fainter and more elongated spots are from the film (either side of central spot).

tilts of detector with respect to beam) were determined by using the $SrTiO_3$ substrate as an unstrained reference. T_c measurements of 90.4 K yielded an O_2 content of 7.0, which was then used to calculate the bulk unstrained lattice parameters as: a = 3.8154 Å, b = 3.8888 Å and c = 11.6764 Å.

We found that the strain values in the $YBa_2Cu_3O_7$ film are on the order of 10^{-2} and the effect of the cubic substrate is to make the $YBa_2Cu_3O_7$ structure look tetragonal rather than orthorhombic. The values are consistent with epitaxial strains due to the difference in lattice parameters of the substrate and the film. Due to the large strain values, automated indexation of the diffraction pattern is not straight forward because of the necessity to use a large angular tolerance. We therefore used as an intermediate unstrained reference quadratic values for the $YBa_2Cu_3O_7$ lattice constants and then compare the refined values with the bulk reference. Figures 2 and 3 give the deviatoric strain along the crystallographic unit cell directions, a and b, averaged for the 10 traverses across the grain boundary in the 36° and 10° tilt samples, respectively.

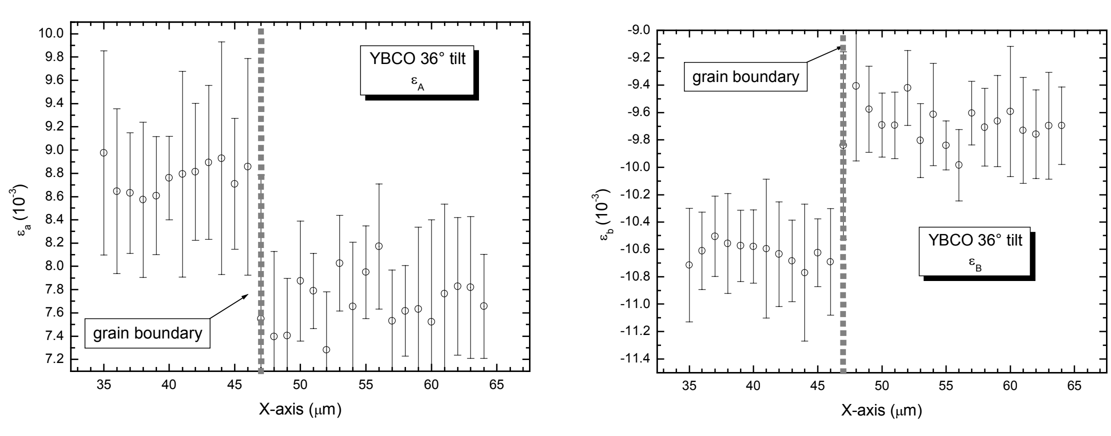


Figure 2. Deviatoric strain measurements along the a-direction (left) and the b-direction (right) of the unit cell averaged over 10 traverses across the grain boundary of the 36° tilt bicrystal.

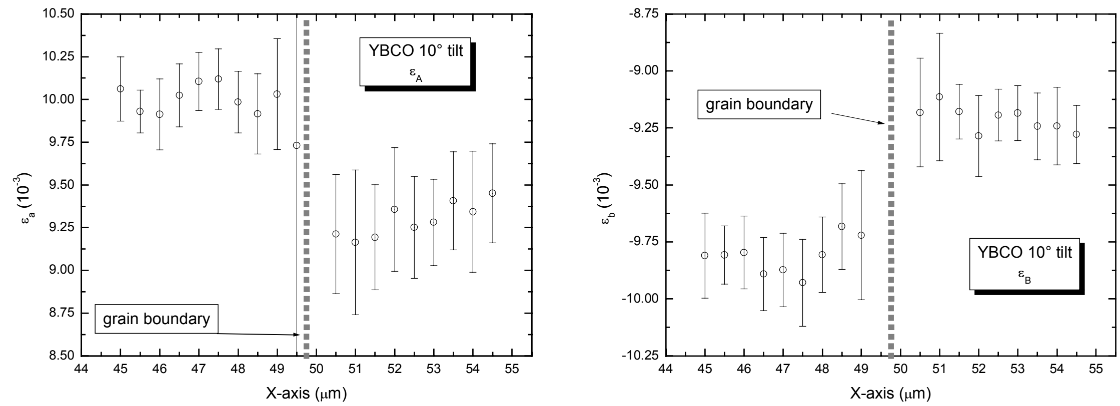


Figure 3. Deviatoric strain measurements along the a-direction (left) and the b-direction (right) of the unit cell averaged over 10 traverses across the grain boundary of the 10° tilt sample.

CONCLUSIONS/DISCUSSION

The deviatoric strain state in the unit cell coordinate system is different on opposing sides of the 36° and 10° bicrystal grain boundary. No strain gradients can be detected within our spatial resolution limit as we approach the grain boundary from either side. Future work will include data collection and analysis at the cryogenic operating conditions of these films.

ACKNOWLEDGMENTS

Thanks to Gertjan Koster and Ted Geballe for providing samples and measuring T_c's.

REFERENCES

1. J. Mannhart and P. Chaudhari, Physics Today **54**, 48 (2001).
2. P. Chaudhari et al., Phys. Rev. Lett. **60**, 1653 (1988).
3. D. Dimos, P. Chaudhari and J. Mannhart, Phys. Rev. B **41**, 4038 (1990).
4. Y. Gao et al., Physica C **174**, 1 (1991).
5. R. G. Munro and H. Chen, J. Am. Ceram. Soc. **79**, 603 (1996).
6. A. A. MacDowell et al., Nucl. Inst. Meth. A **467**, 936 (2001).

This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences Division, of the US Department of Energy under Contract No. DE-AC03-76SF00098 at Lawrence Berkeley National Laboratory.

Principal investigator: Wendel (Sander) Caldwell, Advanced Light Source, Ernest Orlando Lawrence Berkeley National Laboratory. Email: WACaldwell@lbl.gov. Telephone: 510-495-2233.